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Energy Levels in Si and SrTiO₃-Based Quantum Wells with Charge Image Effects

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In the present work we develop a theoretical study to analyze how the image charges effects can modify the electronic properties in Si and SrTiO₃-based quantum wells. We have used the method based on the calculation of the image charge potential by solving Poisson equation in cylindrical coordinates. The numerical results show that the electron-heavy hole recombination energy can be shifted by more than 200 meV due to the combination of charge image and SiO₂ (SrTiO₃) interface thickness effects.

Keywords: Energy Levels; Si; SrTiO₃-based quantum wells

I. INTRODUCTION

The SiO₂ gate thickness shrinkage to less than 50 Å is driving research efforts to find alternative oxides with high dielectric constant to allow for physically thicker films that can limit leakage current problems [1]. Recent research shows that SrTiO₃, HfO₂ and TiO₂ materials are the most promising candidates to SiO₂ replacement in development of new semiconductors devices. With the advances in the growth of SrTiO₃ on silicon by epitaxy [2], the development of quantum confinement based optical devices is possible, following the steps of an original suggestion and demonstration of light emission in Si/SiO₂ quantum wells (QWs) [3, 4], by simple replacement of silicon dioxide by SrTiO₃. The understanding of the atomic structure at the silicon/oxide interface is still not complete. However, the ability to grow gate quality crystalline oxide films on Si in industrial scale is yet to be demonstrated. Droopad *et al.* [5] observed that the possible explanation for the formation of such an amorphous layer includes the diffusion of oxygen during the growth of the oxide layer reacting with the interfacial Si atoms. This would suggest that the interface layer is some form of SiO_x with $x \leq 2$. Chambers *et al.* [6] have shown that the interest in including an interfacial layer of SiO₂ suggests significant progress in order to reduce the leakage current, either because SiO₂ acts as an electron tunnel barrier or because SiO₂ at the interface increases the conduction band offset between SrTiO₃ and Si. Tuan *et al.* [7] show that the TiO₂ can not be grown directly on Si because of thermodynamic instabilities, leading to TiSi_x and SiO₂ at the interface. However, TiO₂ can be grown as an epitaxial film on SrTiO₃ (001) that can be grown epitaxially on Si(001) with negligible interface reaction.

In this work, we present results on electron-hole energy recombination from confined states in abrupt Si/SiO₂/SrTiO₃ and Si/SrTiO₃/TiO₂ QWs. The aim is to search for high-*k* dielectric based light emission devices, which can be important in developing silicon-based technology for future nanophotonic device integration. The dielectric mismatches among the materials of QWs are included through the conventional image potential for a point charge *Q* near an interface [8].

II. THEORETICAL MODEL

The carrier Hamiltonian in Si and SrTiO₃-based quantum wells can be written as

$$H(z) = -\frac{\hbar^2}{2} \frac{d}{dz_i} \left(\frac{1}{m_i} \frac{d}{dz_i} \right) + V_T(z), \quad (1)$$

with *i* = electron or hole and the total effective potential *V_T*(*z*) given by

$$V_T(z) = V_0(z) + V_{im}(z), \quad (2)$$

where *V₀*(*z*) is the potential energy due to the conduction (or valence) band offset and *V_{im}*(*z*) is the image charge potential contribution, given by the Poisson's equation due to the presence of a point charge

$$\vec{\nabla} \cdot [\epsilon(z) \vec{\nabla} \phi(\vec{r})] = -Q\delta(\vec{r} - \vec{r}_0). \quad (3)$$

The solution in the cylindrical coordinates is independent of the azimuth angle ϕ (see detail in Ref. [8]). In this case, we can write $\phi(\vec{r})$ in the general form

$$\phi(\vec{r}) = \int_0^\infty q J_0(qR) A_q(z) dq, \quad (4)$$

where *J₀*(*qR*) is the Bessel function of the zeroth order, *A_q*(*z*) is a function determined by the boundary conditions of $\phi(\vec{r})$ at the interfaces. The solution for the image potential *V_{im}*(*z*) is

$$V_{im}(z_0) = \frac{Q}{2} \int_0^\infty q [A_q(z_0) - A_q^0(z_0)] dq, \quad (5)$$

where *A_q*⁰(*z*₀) is solution of (3) if the dielectric constant were *z* independent.

Using the above considerations, we solved the Schrödinger equation for the perpendicular motion:

$$H_i(z_i)\psi_i(z_i) = E_i^n \psi_i(z_i) \quad (6)$$

and the eigenvalues and eigenfunctions of this equation are calculated through a matrix transfer scheme [9].

III. NUMERICAL RESULTS

The heterostructures used in our simulations have been a $TiO_2/SrTiO_3/Si$ and $SrTiO_3/SiO_2/Si$ QW. All the parameters used for $SrTiO_3$, SiO_2 , TiO_2 and Si are presented in Table I.

TABLE I: Parameters of the materials used in our theoretical calculations [10-12].

	<i>Si</i>	<i>SiO₂</i>	<i>SrTiO₃</i>	<i>TiO₂</i>
E_g (eV)	1.1	8.9	3.3	3.2
ϵ/ϵ_0	11.7	2.1	300	100
$m_{e,\perp}/m_0$	0.173	0.3	0.676	0.3454
$m_{h,\perp}/m_0$	0.533	5.0	1.588	5.0208

In the present calculation two effects are considered, the charge image and the interface thickness. Fig. 1 shows the confinement potential $V_T(z)$ and the wave functions of $TiO_2/SrTiO_3/Si$ (left) and $SrTiO_3/SiO_2/Si$ (right) heterostructures with quantum well width of 5.0 nm and SiO_2 ($SrTiO_3$) layers with thickness of 1.0 nm.

Considering $TiO_2/SrTiO_3/Si$ system, and based on the work of Tuan *et al.* [7], the conduction band offset of 0.1 eV and 0.2 eV between Si and $SrTiO_3$ and between Si and TiO_2 , respectively were used – see Fig. 1 (left). In this structure the attractive character of the image charges in the well region introduce a sharp and deep potential profile which can trap carriers close to the $SrTiO_3/Si$ interfaces. This fact can be seen looking through the top of electron wave function evolution in Fig. 2 (left).

For $SrTiO_3/SiO_2/Si$ systems electron confinement was not observed if we consider a band offset of 0.1 eV between $SrTiO_3$ and Si . In this structure we have used a band offset of 0.9 eV, as proposed by Zang *et al.* [13]. Thus, as shown in Fig. 1 (right), there are two confined states for electrons and four confined states for heavy hole in a narrow QW with width of 5.0 nm. We also observed that in this system the SiO_2/Si interface does not permit interfacial confinement due to the repulsive character of the image charge in the well region – see Fig. 2 (right).

Figure 3 shows the results for electron-heavy hole recombination energy in $TiO_2/SrTiO_3/Si$ QW (top) and $SrTiO_3/SiO_2/Si$ QW (bottom), as function of the QW width for $SrTiO_3$ (SiO_2) layer with thickness of 1.0 nm and 1.5 nm. Solid and dashed lines represent carrier recombination energy including the effects due to image charges.

Dashed dotted and dotted lines represent carrier recombination energy without image charges effects. The attractive character of the image potential in the well region of

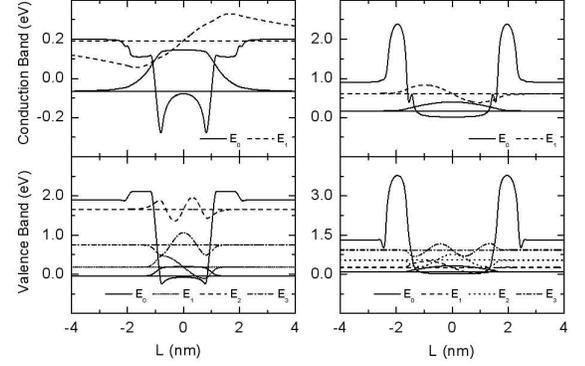


FIG. 1: Confinement $V(z) = V_0(z) + V_{im}(z)$ potentials for 50 Å wide $TiO_2/SrTiO_3/Si$ (left) and $SrTiO_3/SiO_2/Si$ (right). Energy levels and wave function are also depicted.

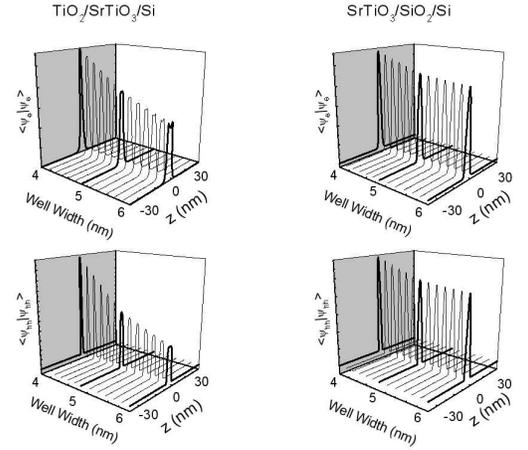


FIG. 2: Electron (top) and heavy hole (bottom) ground states wave functions confined in abrupt $TiO_2/SrTiO_3/Si$ and $SrTiO_3/SiO_2/Si$ QWs, with well width of 4 to 6 nm.

$TiO_2/SrTiO_3/Si$ QW, Fig. 3 (top), decreases the recombination energy (solid and dashed lines), when compared with carrier recombination energy in QW without image charge effect (dashed dotted and dotted lines). The repulsive image potential in the well region of $SrTiO_3/SiO_2/Si$ QW, Fig. 3 (bottom), increases the recombination energy. The $SrTiO_3$ (SiO_2) layer is expressive because it strongly affects the recombination energy of the QWs. Fig. 3 also shows that increasing the thickness of the $SrTiO_3$ (SiO_2) layer, the recombination energy blue-shift in $TiO_2/SrTiO_3/Si$ by about 40 meV and in $SrTiO_3/SiO_2/Si$ by about 800 meV, respectively, for a well width of 4.0 nm.

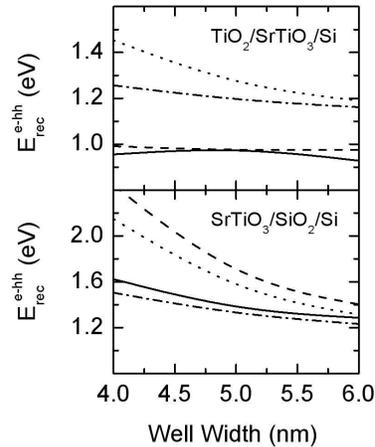


FIG. 3: Electron-heavy hole recombination energy in (top) $TiO_2/SrTiO_3/Si$ and (bottom) $SrTiO_3/SiO_2/Si$, as a function of the well width and $SrTiO_3$ (SiO_2) layer with thickness of 1.0 nm (solid and dashed dotted lines) and 1.5 nm (dashed and dotted lines).

In conclusion, we have studied image charges effects in $TiO_2/SrTiO_3/Si$ and $SrTiO_3/SiO_2/Si$ QWs. The image charges related potential structure (sharp and deep) can trap electrons close to the $SrTiO_3/Si$ interfaces. In this system we also observed that the attractive character of the image potential inside of the well region decreases the recombination energy. For $SrTiO_3/SiO_2/Si$ QW we observed electron confinement only for a 0.9 eV conduction band offset between the $SrTiO_3$ and Si layers. This structure does not have a sharp and deep potential profile due to the repulsive character of the image potential that increases the recombination energy, consequently the carrier do not presents an interfacial confinement.

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